

Appendix A



FIGURE 1 (CONT.)

	_	- AMAZIA							
MOTA	1912	0	ASP	319	82.640	80.353	71.870	1.00	16.26
MOTA	1913	N	ALA	320	80.593	81.055	72.464	1.00	11.91
ATOM	1914	CA	ALA	320	80.102	79.758	72.914	1,00	7.79
MOTA	1915	CB	ALA	320	80.830	79.315	74.163	1.00	3.09
MOTA	1916	C	ALA	320	78.632	79.953	73.218	1.00	8.10
MOTA	1917	0	ALA	320	78.165	81.092	73.284	1.00	9.40
MOTA	1918	N	LEU	321	77.900	78.856	73.404	1.00	8.90
MOTA	1919	CA	LEU	321	76.467	78.917	73.713	1.00	6.89
MOTA	1920	СВ	LEU	321	75.645	78.427	72.529	1.00	2.00
MOTA	1921	CG	LEU	321	75.538	79.283	71.268	1.00	2.00
MOTA	1922	CD1	LEU	321	75.062	78.394	70.158	1.00	4.37
ATOM	1923	CD2	LEU	321	74.589	80.461	71.444	1.00	2.00
MOTA	1924	C	LEU	321	76.121	78.088	74.947	1.00	8.16
ATOM	1925	0	LEU	321	76.665	77.008	75.144	1.00	10.39
MOTA	1926	N	ARG	322	75.258	78.618	75.804	1.00	7.97
ATOM	1927	CA	ARG	322	74.836	77.907	77.001	1.00	7.47
MOTA	1928	CB	ARG	322	74.697	78.883	78.168	1.00	9.30
ATOM	1929	CG	ARG	322	74.550	78.234	79.535	1.00	15.10
ATOM	1930	CD	ARG	322	74.657	79.288	80.642	1.00	18.83
ATOM	1931	NE	ARG	322	74.309	78.765	81.965	1.00	18.29
ATOM	1932 1933	CZ NH1	ARG	322	73.750	79.488	82.932	1.00	17.03
ATOM			ARG	322	73.483	80.771	82.740 84.079	1.00	18.79
MOTA MOTA	1934 1935	NH2 C	ARG ARG	322	73.411 73.486	78.921	84.078	1.00	16.70
ATOM	1936	ŏ	ARG	322 322	73. 4 66 72.535	77.329 78.071	76.602	1.00	8.75
ATOM	1937	N	VAL	323	72.535 73.424	76.071 76.012	76.373 76.455	1.00 1.00	10.16 8.83
ATOM	1938	CA	VAL	323	73.424 72.209	75.346	76.433 76.023	1.00	10.03
ATOM	1939	СВ	VAL	323	72.523	74.365	76.023 74.871	1.00	9.77
ATOM	1940	CG1	VAL	323	71.306	74.565 73.549	74.507 74.507	1.00	16.85
ATOM	1941	CG2	VAL	323	72.993	75.5≈3 75.137	73.653	1.00	7.40
ATOM	1942	C	VAL	323	71.473	74.633	73.033 77.153	1.00	13.18
ATOM	1943	ŏ	VAL	323	72.053	73.803	77.853	1.00	15.10
ATOM	1944	Ň	GLY	324	70.196	74.969	77.327	1.00	12.40
ATOM	1945	CA	GLY	324	69.392	74.347	78.362	1.00	13.80
MOTA	1946	C	GLY	324	68.211	75.201	78.791	1.00	14.53
MOTA	1947	0	GLY	324	68.367	76.397	78.997	1.00	17.39
ATOM	1948	N	MET	325	67.026	74.613	78.901	1.00	11.83
MOTA	1949	CA	MET	325	65.868	75.368	79.341	1.00	13.08
MOTA	1950	СВ	MET	325	65.201	76.124	78.186	1.00	12.41
ATOM	1951	CG	MET	325	64.150	77.118	78.678	1.00	10.52
MOTA	1952	SD	MET	325	63.227	78.025	77.440	1.00	13.36
MOTA	1953	CE	MET	325	62.495	79.307	78.488	1.00	7.16
MOTA	1954	С	MET	325	64.829	74.561	80.130	1.00	15.26
MOTA	1955	0	MET	325	64.051	73.781	79.563	1.00	15.50
MOTA	1956	N	GLY	326	64.848	74.751	81.447	1.00	15.85
MOTA	1957	CA .	GLY	326	63.899	74.093	82.323	1.00	17.08
MOTA	1958	C	GLY	326	64.165	72.651	82.677	1.00	18.22
MOTA	1959	0	GLY	326	63.270	71.957	83.148	1.00	18.82
MOTA	1960	N	CYS	327	65.401	72.206	82.515	1.00	20.56
MOTA	1961	CA	CYS	327	65.746	70.823	82.821	1.00	22.33
ATOM	1962	СВ	CYS	327	66.443	70.194	81.622	1.00	20.50
MOTA	1963	SG	CYS	327	67.878	71.121	81.089	1.00	21.45
MOTA	1964	C	CYS	327	66.633	70.710	84.061	1.00	24.86
MOTA	1965	0	CYS	327	66.992	69.597	84.487	1.00	26.55
ATOM .	1966	N	GLY	328	67.007	71.859	84.619	1.00	23.64
MOTA MOTA	1967	CA	GLY	328	67.846	71.867	85.802	1.00	23.90
ATOM	1968 1969	C O	GLY	328	67.066 65.043	71.347	86.988 87.468	1.00	23.07
AT ON	1303	J	GLY	328	65.913	71.735	87.168	1.00	23.22

FIGURE 1 (CONT.)

ATOM	1970	N	SER	329	67.706	70.528	87.822	1.00	23.68
ATOM	1971	CA	SER	329	67.077	69.925	89.000	1.00	22.19
ATOM	1972	СВ	SER	329	68.150	69.406	89.964	1.00	19.55
ATOM	1973	OG	SER	329	69.028	70.440	90.356	1.00	23.14
ATOM	1974	C	SER	329	66.077	70.812	89.747	1.00	23.28
		Ö	SER	329	64.978	70.362	90.065	1.00	25.72
ATOM	1975			330		70.302 72.070	89.992	1.00	22.81
ATOM	1976	N	ILE		66.444			1.00	19.85
ATOM	1977	CA	ILE	330	65.584	73.024	90.700		
MOTA	1978	СВ	ILE	330	66.410	74.017	91.589	1.00	15.67
MOTA	1979	CG2	ILE	330	66.509	73.500	93.001	1.00	18.25
MOTA	1980	CG1	ILE	330	67.795	74.289	90.994	1.00	7.11
MOTA	1981	CD1	ILE	330	67.776	74.921	89.639	1.00	5.46
MOTA	1982	С	ILE	330	64.703	73.869	89.786	1.00	20.60
MOTA	1983	0	ILE	330	64.225	74.923	90.201	1.00	23.53
MOTA	1984	N	IMP	331	64.425	73.400	88.579	1.00	19.32
MOTA	1985	CA	IMP	331	63.641	74.206	87.649	1.00	20.33
MOTA	1986	С	IMP	331	62.148	73.909	87.498	1.00	21.39
MOTA	1987	0	IMP	331	61.737	72.757	87.342	1.00	22.62
MOTA	1988	CB	IMP	331	64.310	74.200	86.277	1.00	19.26
ATOM	1989	SG	IMP	331	64.038	75.775	85.516	1.00	16.83
MOTA	1990	P	IMP	331	71.205	71.206	87.339	1.00	24.40
ATOM	1991	01P	IMP	331	70.381	70.028	86.885	1.00	22.40
ATOM	1992	O2P	IMP	331	72.615	71.144	86.864	1.00	18.66
ATOM	1993	03P	IMP	331	71.172	71.333	88.803	1.00	19.75
ATOM	1994	O5°	IMP	331	70.688	72.534	86.798	1.00	22.96
ATOM	1995	C5*	IMP	331	71.500	73.726	87.024	1.00	14.95
ATOM	1996	C4°	IMP	331	71.156	74.601	85.831	1.00	11.32
MOTA	1997	O4*	IMP	331	69.758	74.898	85.861	1.00	12.20
	1998	C3*	IMP	331	71.865	75.962	85.934	1.00	12.62
MOTA		O3*	IMP	331	73.078	76.011	85.208	1.00	10.24
MOTA	1999		IMP	331	70.883	76.903	85.210	1.00	13.74
MOTA	2000	C2*			70.863 70.752	76.903 76.706	83.816	1.00	13.7 ⊈ 11.66
MOTA	2001	O2*	IMP	331				1.00	14.52
ATOM	2002	C1°	IMP	331	69.602	76.308	85.761 86.642		18.13
MOTA	2003	N9	IMP	331	68.832	77.205	86.612 87.500	1.00	
MOTA	2004	C8	IMP	331	69.321	78.030	87.599	1.00	18.02
MOTA	2005	N7	IMP	331	68.331	78.568	88.322	1.00	16.06
MOTA	2006	C5	IMP	331	67.170	78.093	87.806	1.00	19.77
MOTA	2007	C6	IMP	331	65.799	78.289	88.156	1.00	22.26
MOTA	2008	06	IMP	331 .	65.412	78.995	89.085	1.00	17.37
MOTA	2009	N1	IMP	331	64.941	77.579	87.374	1.00	25.96
MOTA	2010	C2	IMP	331	65.296	76.706	86.299	1.00	23.29
MOTA	2011	N3	IMP	331	66.567	76.524	85.957	1.00	24.20
MOTA	2012	C4	IMP	331	67.498	77.200	86.693	1.00	21.15
MOTA	2013	N	ILE	332	61.333	74.959	87.564	1.00	19.04
MOTA	2014	CA	ILE	332	59.899	74.811	87.391	1.00	18.02
MOTA	2015	CB	ILE	332	59.071	75.097	88.696	1.00	16.99
MOTA	2016	CG2	ILE	332	59.423	74.093	89.793	1.00	12.90
MOTA	2017	CG1	ILE	332	59.283	76.525	89.191	1.00	14.79
ATOM	2018	CD1	ILE	332	58.212	77.005	90.159	1.00	8.04
MOTA	2019	С	ILE	332	59.401	75.675	86.226	1.00	20.21
ATOM	2020	Ö	ILE	332	58.195	75.848	86.050	1.00	21.52
ATOM	2021	Ň	THR	333	60.330	76.195	85.420	1.00	20.15
ATOM	2022	CA	THR	333	59.993	77.020	84.251	1.00	19.79
ATOM	2023	СВ	THR	333	61.287	77.491	83.467	1.00	20.47
ATOM	2024	0G1	THR	333	61.948	78.537	84.191	1.00	18.21
MOTA	2025	CG2	THR	333	60.949	70.337 77.996	82.058	1.00	16.88
ATOM	2025	C	THR	333	59.060	76.275	83.281	1.00	18.99
								1.00	
MOTA	2027	0	THR	333	58.124	76.861	82.737	1.00	19.34